

Importance of Mineralogical Data for Groundwater Quality Affected by CO₂ Leakage from Storage Sites

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International Symposium on Site Characterization for CO₂
Geological Storage

March 20-22, 2006; Berkeley, California

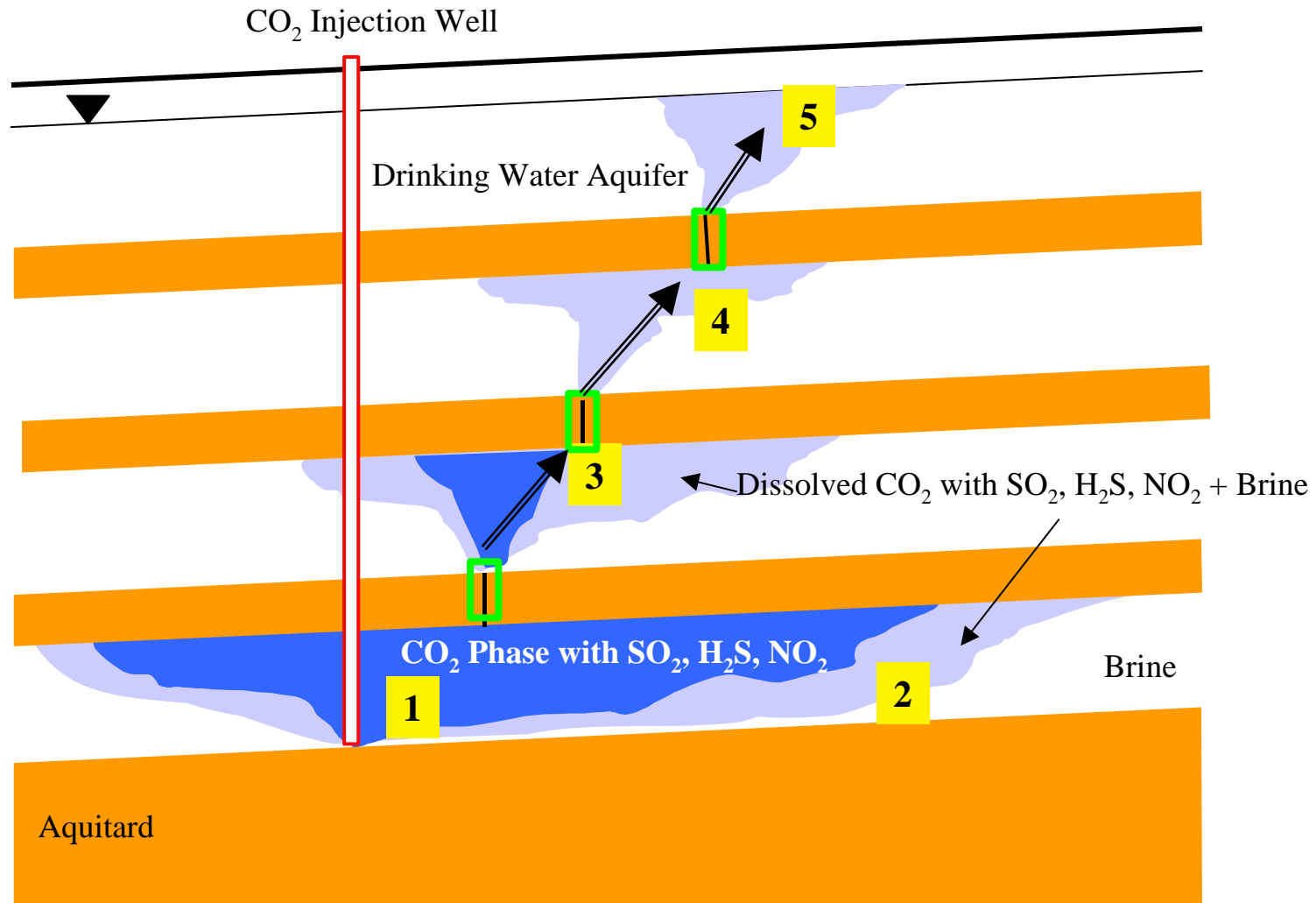
- Introduction
- Problem Setup
- Numerical Simulator
- Results
- Conclusions

INTRODUCTION



- The impact of leakage from CO₂ storage reservoirs on groundwater quality is one of the concerns.
- Dissolution of CO₂ in groundwater results in a decrease in pH.
- Such acidic condition can affect the dissolution and sorption mechanisms of many minerals such as galena (PbS).
- If calcite is present in the rock, it can buffer the pH and reduce galena dissolution.
- Insight into which minerals and compounds are most important for groundwater quality can be obtained from reactive geochemical transport simulations.

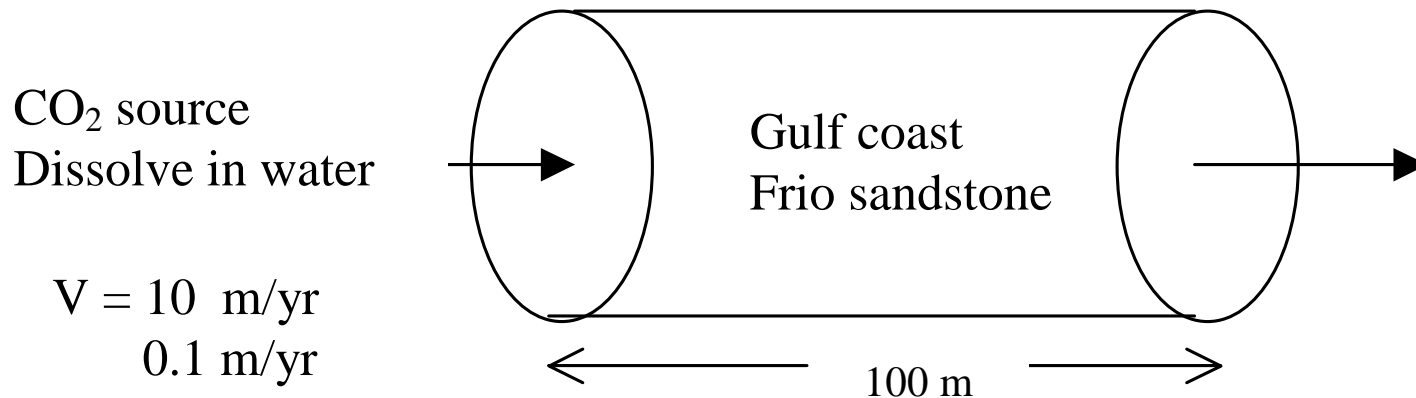
PROBLEM SETUP (1)



PROBLEM SETUP (Flow)



- Before conducting site-specific investigations, it is necessary to explore features in a generic manner.
- A 1-D system of 100 m length was used for studying water quality evolution.



PROBLEM SETUP (Water Chemistry)



- A separate CO_2 phase could exist in the CO_2 source zone.
- For purpose of water quality studies, we assumed acid gas dissolution into 1 M NaCl brine with
 - CO_2 , a partial pressure of 100 bar
 - H_2S , 1 bar
 - SO_2 , 10^{-4} bar
- The resulting source water has
 - a pH of about 3
 - a dissolved inorganic carbon concentration of 1.54 mol/kg
 - a dissolved sulfur of 0.15 mol/kg
- An injected CO_2 stream may contain other constituents such as NO_x and mercury that were not considered.

PROBLEM SETUP (Mineralogy)



- We started from a Gulf Coast Frio sandstone (right).
- Calcite and anhydrite are assumed to react at equilibrium.
- Other mineral reactions proceed under kinetic conditions.
- A general kinetic rate law accounting for multiple mechanisms was used.

Mineral	Vol.% Of solid	A (cm ² /g)
Primary:		
Quartz	57.888	9.8
Kaolinite	2.015	151.6
Calcite	1.929	
Illite	0.954	151.6
Oligoclase	19.795	9.8
K-feldspar	8.179	9.8
Na-smectite	3.897	151.6
Chlorite	4.556	9.8
Hematite	0.497	12.9
Secondary:		
Anhydrite		
Magnesite		9.8
Dolomite		9.8
Low-albite		9.8
Siderite		9.8
Ankerite		9.8
Dawsonite		9.8
Ca-smectite		151.6
Alunite		9.8
Pyrite		12.9

PROBLEM SETUP (Simulations)



➤ List of simulations

Simulation	Pore velocity, m/y)	Mineralogy
1	10	Frio sandstone with a volume of calcite 2%; Basis case
2	10	No calcite
3	10	Double calcite
4	0.1	Same as simulation 1
5	10	Pb, Zn bearing minerals, galena and sphalerite

➤ Changes of abundances of calcites, galena and sphalerite are adjusted with abundance of quartz.

Processes:

- Multiphase fluid and heat **flow**: TOUGH2 V2 (Pruess, et al., 1999)
- **Transport**: advection and diffusion in both liquid and gas phases
- Chemical **reactions**:
 - Aqueous complexation
 - Acid-base
 - Redox
 - Mineral dissol./precip. (equilibrium and/or kinetics)
 - Gas dissol./exsol.
 - Cation exchange
 - Surface complexation
 - Linear K_d adsorption
 - Decay

Features:

- Changes in porosity and permeability, and unsaturated zone properties due to mineral dissolution and precipitation
- Gas phase and gaseous species are active in flow, transport, and reaction
- Pitzer and Debye-Hückel activity coefficient models
- A number of chemical species
- CO₂ solubility dependence on P, T and salinity
- Two types of thermodynamic database including EQ3/6 (Wolery, 2004)
- Wide range of conditions
- Publicly available (DOE Software Center)
- <http://esd.lbl.gov/TOUGHREACT/>

TOUGHREACT User's Guide: A Simulation Program for Non-isothermal Multiphase Reactive Geochemical Transport in Variably Saturated Geologic Media

Tianfu Xu, Eric Sonnenthal, Nicolas Spycher and Karsten Pruess

August 2004

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Related CO₂ Geosequestration Papers



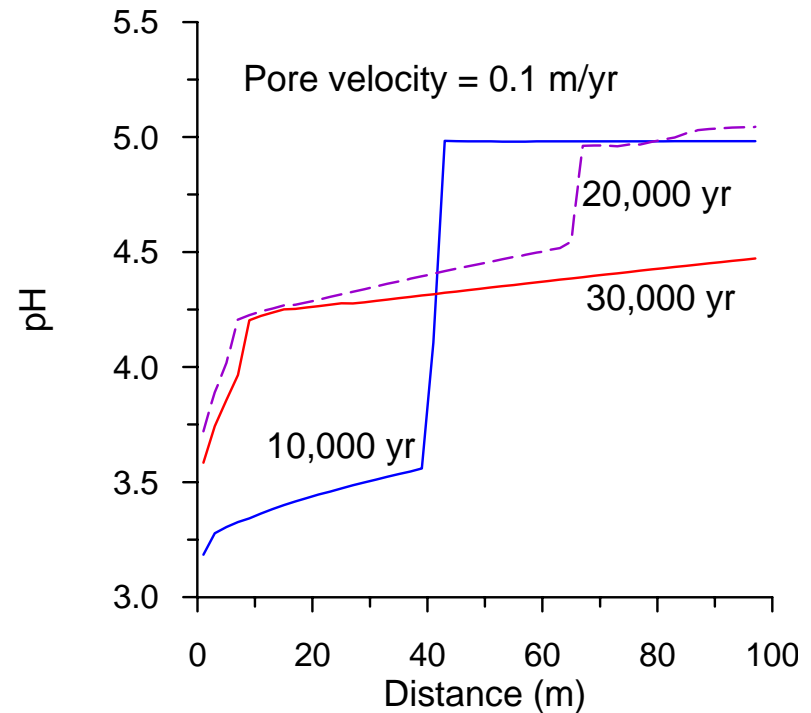
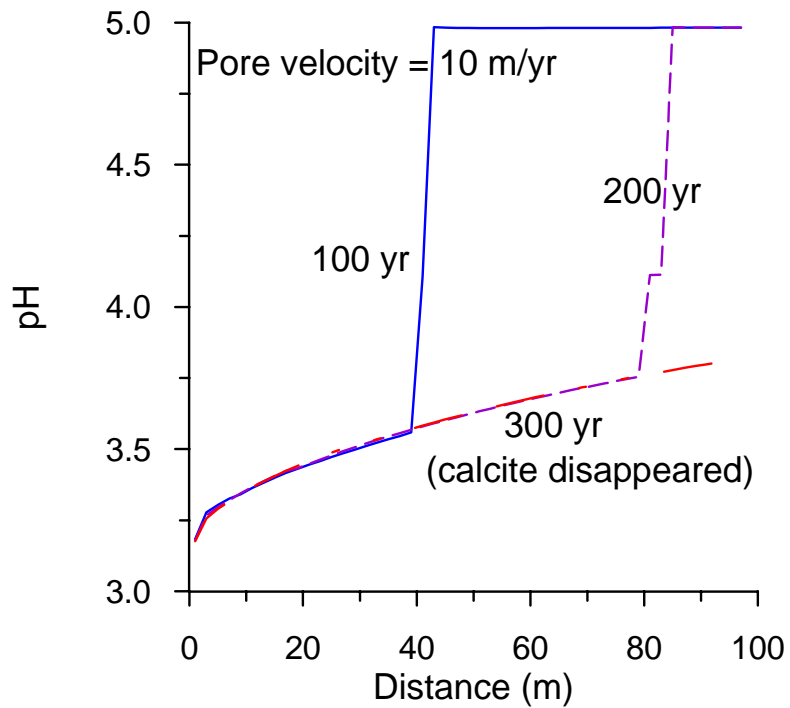
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- Audigane, P., Gaus, I., Czernichowski-Lauriol, I., Pruess, K., Xu, T., Two-dimensional reactive transport modelling of CO₂ injection in a saline aquifer at the **Sleipner site**, submitted to *American Journal of Science*, 2006. (BRGM)

Training Courses

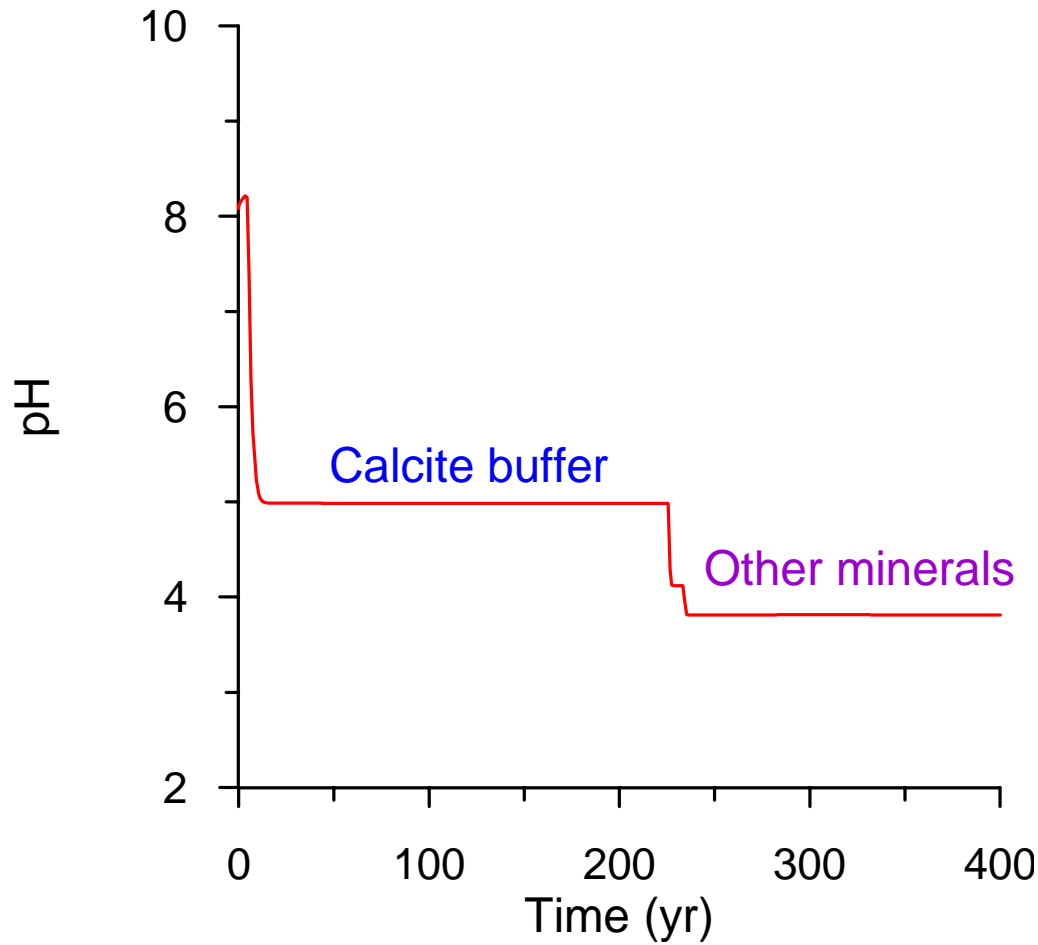


- A short course on TOUGHREACT for 3 days on January 17 - 19, 2006 was offered at LBNL (<http://esd.lbl.gov/TOUGHREACT/training06/index.html>)
- Next Course will be likely in the second week of the coming October
- Email to Tianfu Xu at Tianfu_Xu@lbl.gov to express your interests

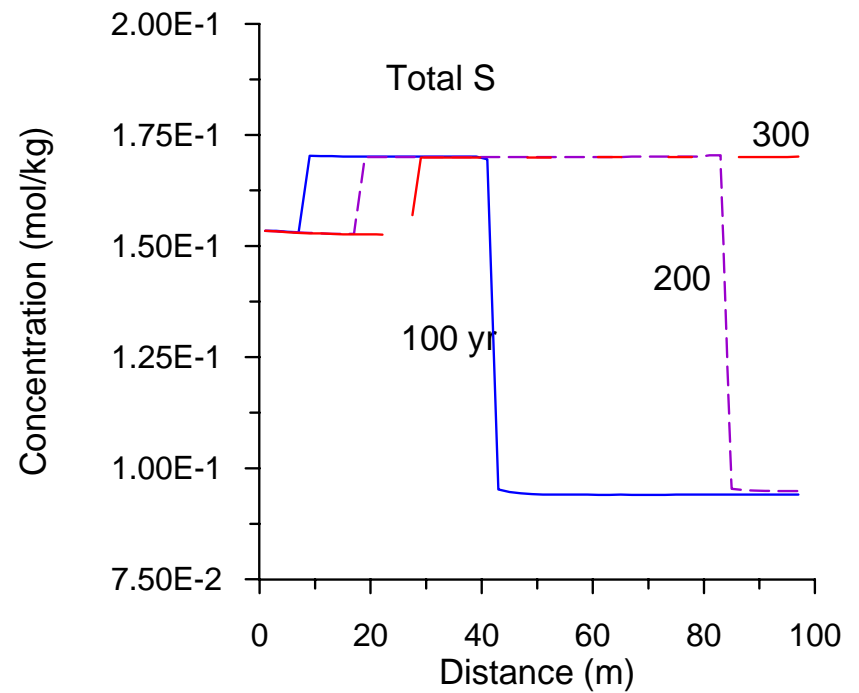
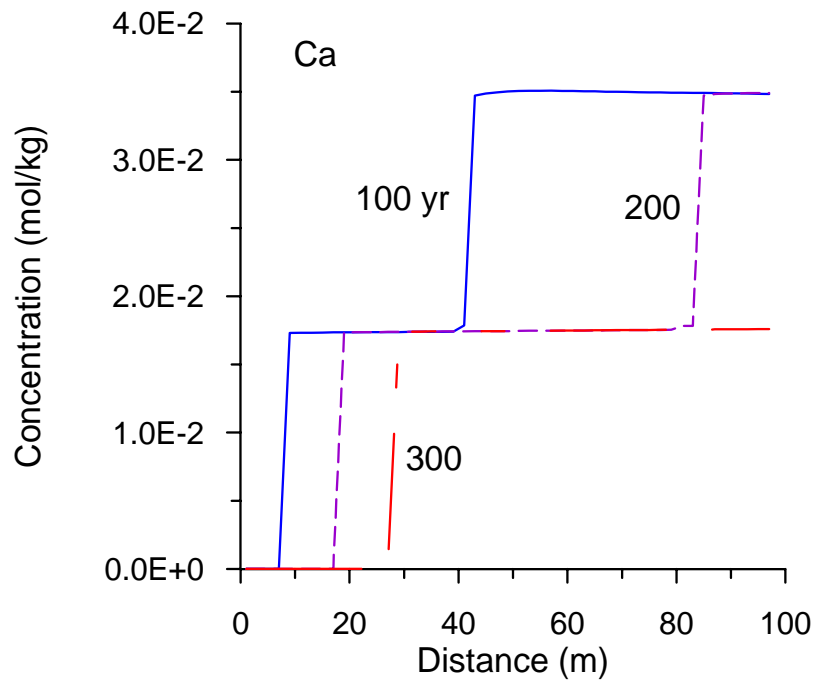
RESULTS (1)



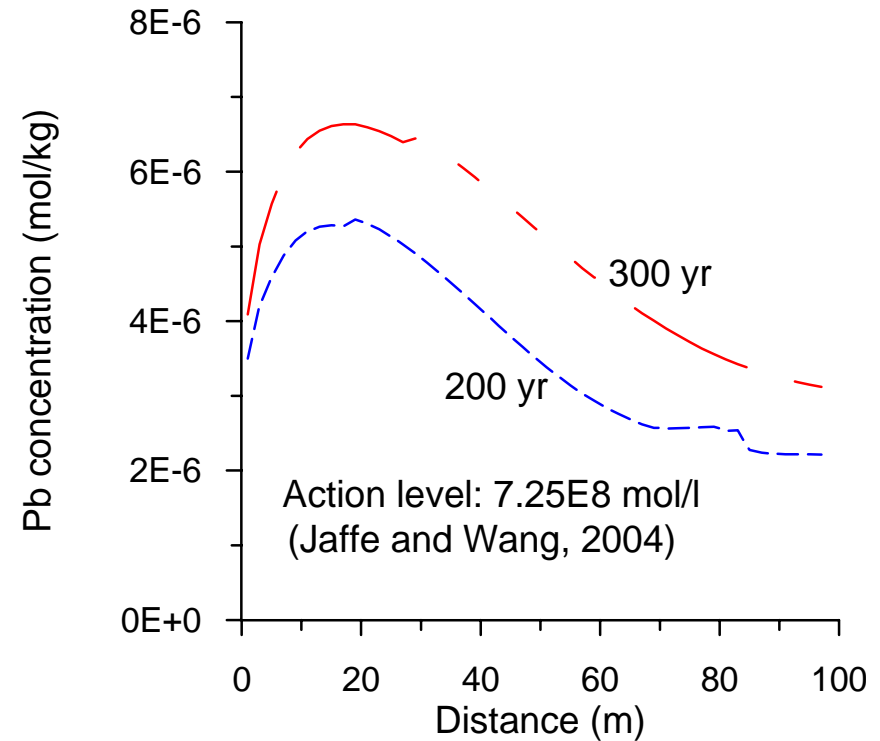
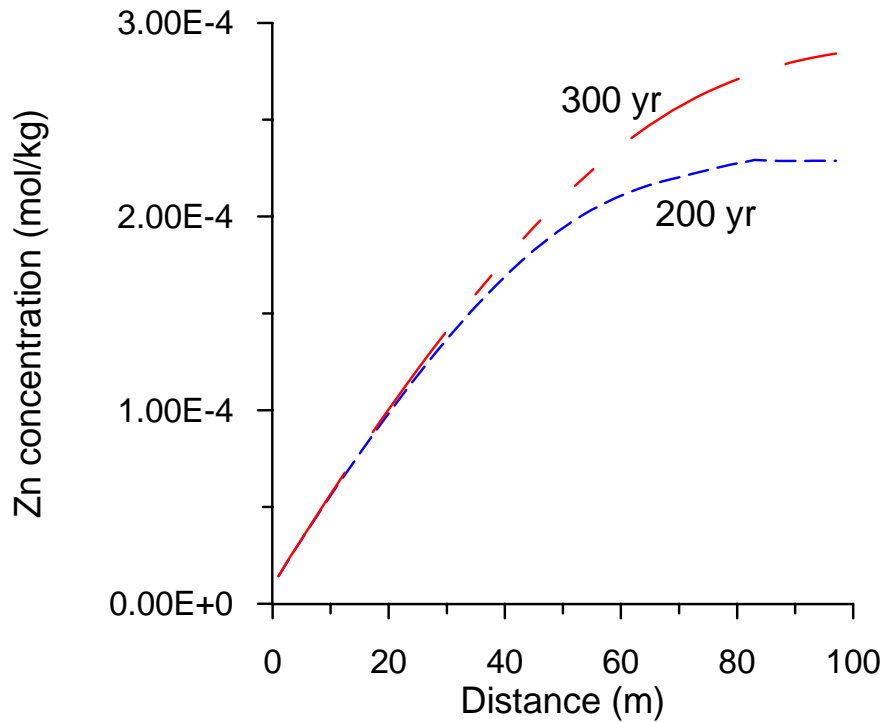
RESULTS (2)



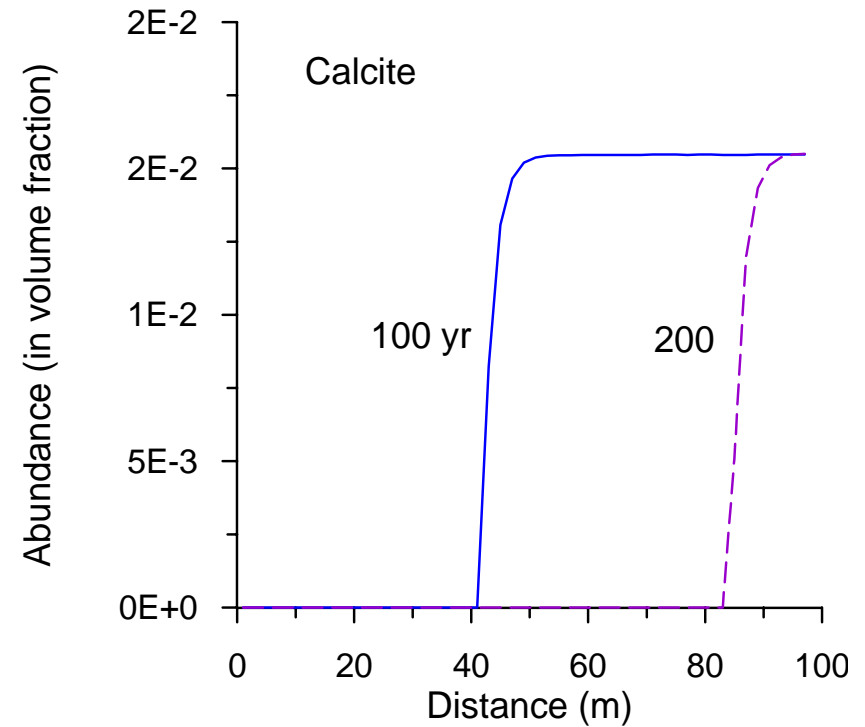
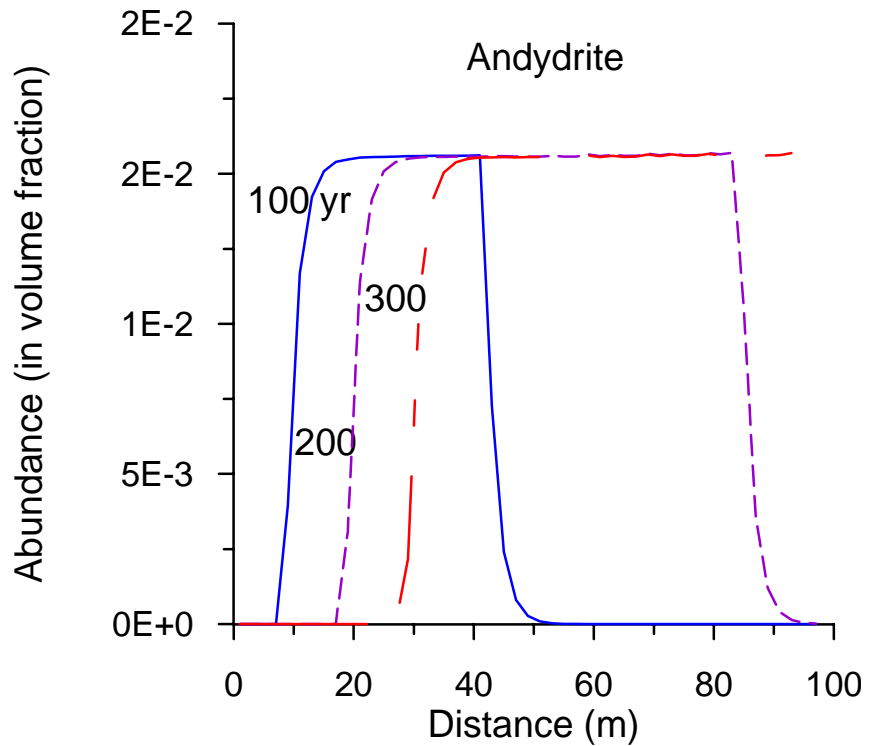
RESULTS (3)



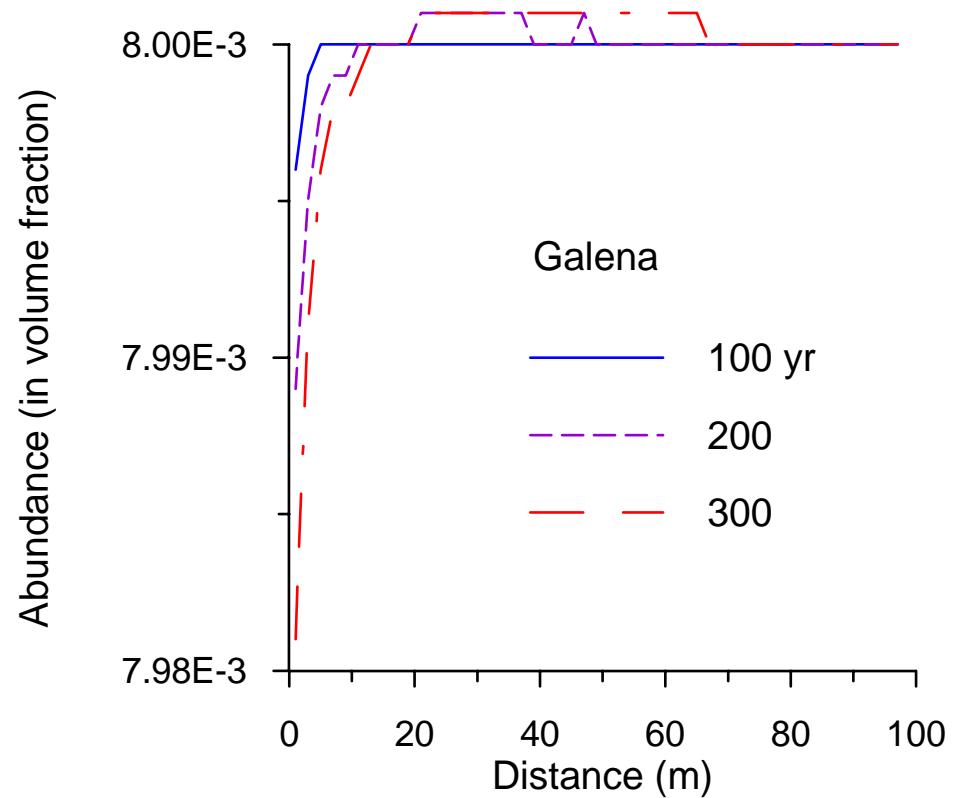
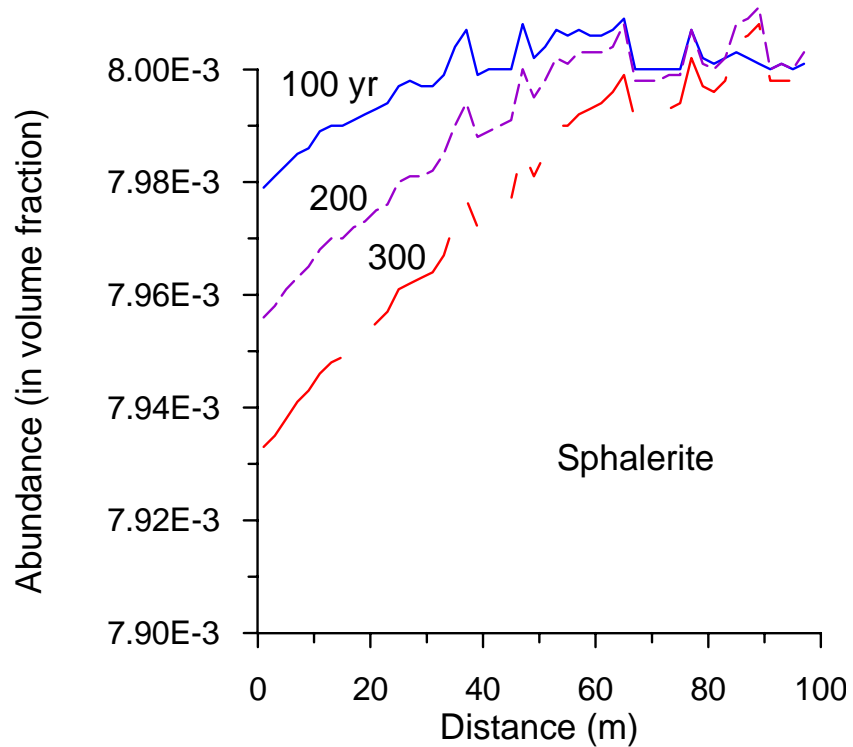
RESULTS (4)



RESULTS (5)



RESULTS (6)



CONCLUSIONS



- Mineralogical data along the CO₂ leakage pathway and in overlying aquifers are important data for water quality evolution, therefore should be an important part of CO₂ site characterization.
- If carbonate minerals such as calcite are present along the leakage pathway, they can buffer the pH to about 5. Other minerals can also buffer the pH but to lesser degree.
- Acidic conditions affect significantly the dissolution and sorption mechanisms of many minerals. For example, if galena is present in the low pH regions its dissolution causes Pb concentration increase much higher than the action level.

ACKNOWLEDGEMENTS



- This work was supported (1) partly by the U.S. Environmental Protection Agency, Office of Water and Office of Air and Radiation under an Interagency Agreement with the U.S. Department of Energy at the Lawrence Berkeley National Laboratory, and (2) partly by the Zero Emission Research and Technology project (ZERT), through Contract number DE-AC02-05CH11231.